



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 01:50 pm GMT

PDB ID : 1OY9
Title : Structural Basis of Multiple Drug Binding Capacity of the AcrB Multidrug Efflux Pump
Authors : Yu, E.W.; McDermott, G.; Zgurskaya, H.I.; Nikaido, H.; Koshland Jr., D.E.
Deposited on : 2003-04-03
Resolution : 3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

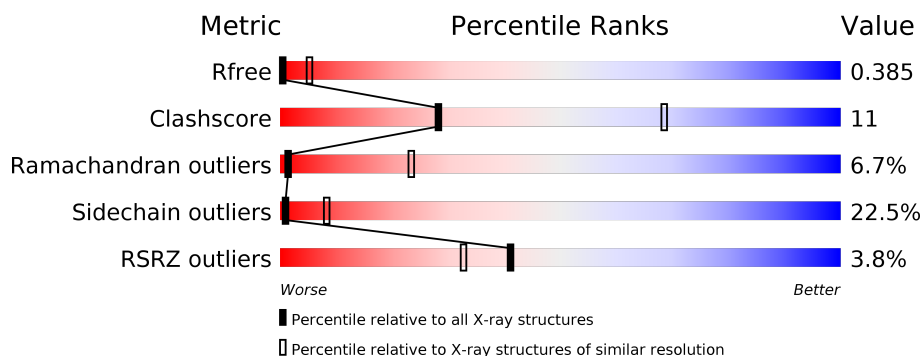
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1019 (4.08-3.52)
Clashscore	112137	1030 (4.04-3.56)
Ramachandran outliers	110173	1011 (4.06-3.54)
Sidechain outliers	110143	1005 (4.06-3.54)
RSRZ outliers	101464	1032 (4.08-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>4%</div> <div>57%</div> <div>31%</div> <div>8%</div> <div>••</div> </div>

2 Entry composition [i](#)

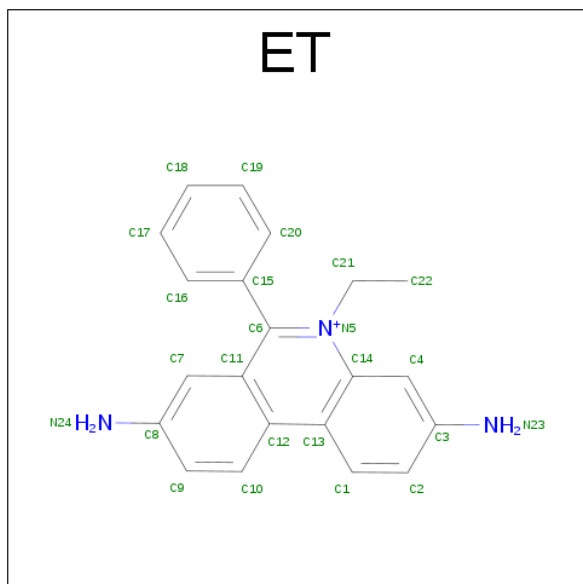
There are 2 unique types of molecules in this entry. The entry contains 7663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1006	Total	C	N	O	S	0	0	0
			7639	4916	1262	1419	42			

- Molecule 2 is ETHIDIUM (three-letter code: ET) (formula: $C_{21}H_{20}N_3$).

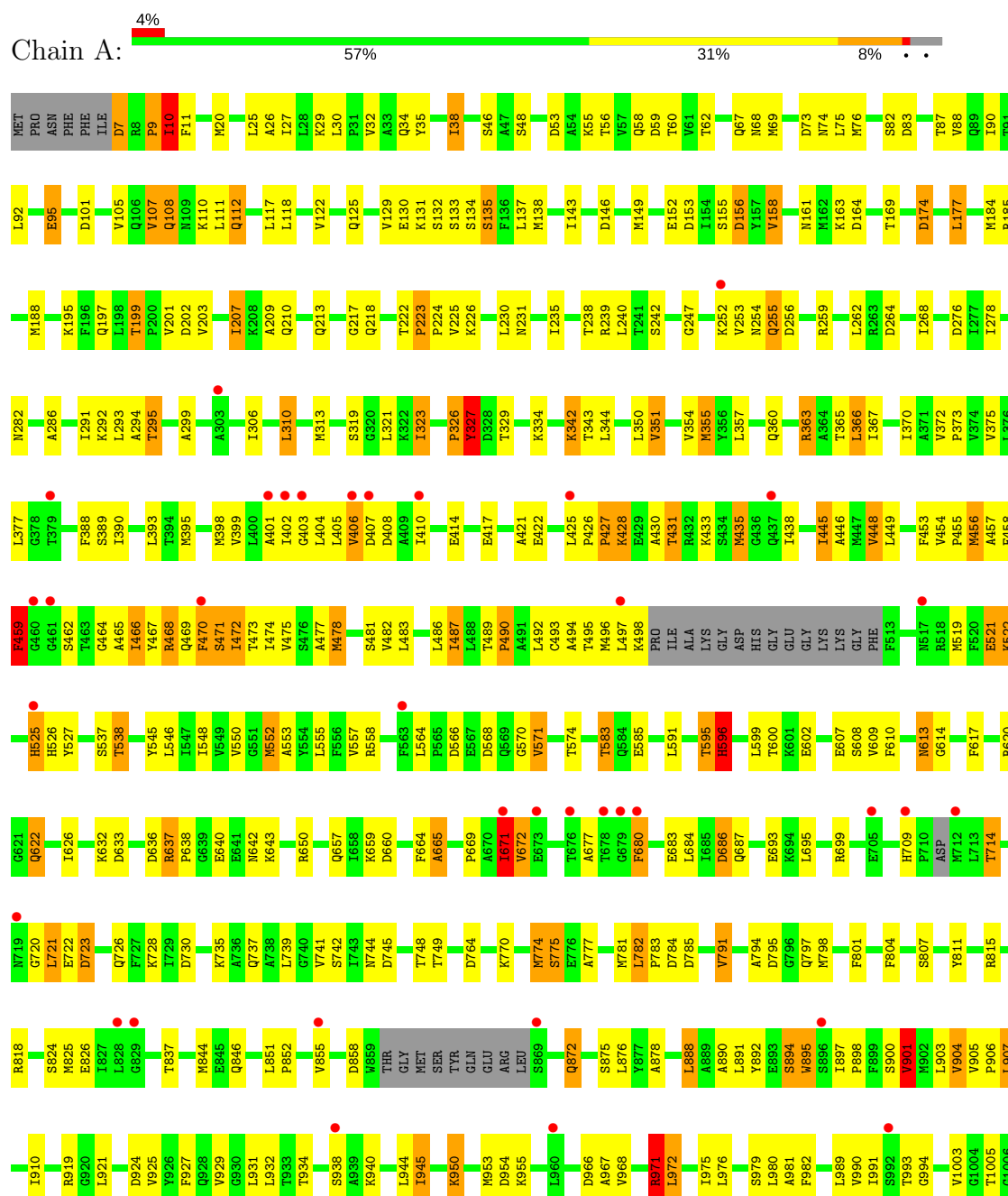


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			24	21	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acriflavine resistance protein B



V1007	M1008	M1011	V1012	T1013	A1014	T1015	V1016	L1017	A1018	I1019	F1020	F1021	V1022	P1023	V1024	F1025	F1026	V1027	V1028	V1029	R1030	R1031	R1032	F1033	S1034	R1035	K1036	ASN	GLU	ASP	ILE	GLU	HIS	SER	HIS	THR	VAL	ASP	HIS	HIS				

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	144.68Å 144.68Å 517.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.60 – 3.80 46.58 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.60-3.80) 84.3 (46.58-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.283 , 0.344 0.376 , 0.385	Depositor DCC
R_{free} test set	1070 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	142.8	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7663	wwPDB-VP
Average B, all atoms (Å ²)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ET

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.43	3/7779 (0.0%)	0.72	38/10563 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	596	HIS	CG-CD2	17.93	1.66	1.35
1	A	596	HIS	CE1-NE2	8.56	1.52	1.32
1	A	596	HIS	CG-ND1	6.96	1.54	1.38

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1032	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	407	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	470	PHE	N-CA-C	6.35	128.15	111.00
1	A	568	ASP	CB-CG-OD2	6.24	123.91	118.30
1	A	723	ASP	CB-CG-OD2	6.21	123.89	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	470	PHE	CA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	A	680	PHE	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7639	0	7800	172	0
2	A	24	0	20	0	0
All	All	7663	0	7820	172	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 172 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ASN:HD22	1:A:613:ASN:C	1.81	0.82
1:A:596:HIS:O	1:A:600:THR:HG22	1.81	0.80
1:A:1022:VAL:HG22	1:A:1023:PRO:HD2	1.65	0.78
1:A:613:ASN:HD22	1:A:614:GLY:N	1.84	0.74
1:A:483:LEU:O	1:A:487:ILE:HG13	1.90	0.72

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	998/1049 (95%)	782 (78%)	149 (15%)	67 (7%)	1	23

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	134	SER
1	A	255	GLN
1	A	327	TYR
1	A	431	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	818/855 (96%)	634 (78%)	184 (22%)	1	8

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	431	THR
1	A	555	LEU
1	A	976	LEU
1	A	435	MET
1	A	478	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	A	391	ASN
1	A	642	ASN
1	A	231	ASN
1	A	657	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ET	A	3001	-	25,27,27	3.02	15 (60%)	33,39,39	1.82	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ET	A	3001	-	-	0/6/6/6	0/4/4/4

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	ET	C6-C11	-2.91	1.38	1.43
2	A	3001	ET	C10-C12	2.10	1.45	1.41
2	A	3001	ET	C17-C16	2.11	1.42	1.38
2	A	3001	ET	C13-C14	2.30	1.45	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	ET	C19-C20	2.36	1.43	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	ET	C7-C11-C6	-3.68	115.87	122.80
2	A	3001	ET	C11-C6-N5	-3.36	114.84	119.10
2	A	3001	ET	C20-C15-C16	-2.57	112.49	117.59
2	A	3001	ET	C19-C20-C15	2.43	123.64	120.57
2	A	3001	ET	C8-C7-C11	3.05	123.71	120.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1006/1049 (95%)	0.12	38 (3%)	41 33	115, 152, 166, 182	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1021	PHE	6.8
1	A	403	GLY	6.0
1	A	679	GLY	5.1
1	A	678	THR	4.7
1	A	497	LEU	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ET	A	3001	24/24	0.68	0.26	-	194,216,226,229	0

6.5 Other polymers [i](#)

There are no such residues in this entry.